

On the binding of small polarons in a mean-field quantum crystal

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We consider a small multi-polaron model obtained by coupling the many-body Schrödinger equation for N interacting electrons with the energy functional of a mean-field crystal with a localized defect, obtaining a highly non linear many-body problem. The physical picture is that the electrons constitute a charge defect in an otherwise perfect periodic crystal. A remarkable feature of such a system is the possibility to form a bound state of electrons via their interaction with the polarizable background. We first prove that a single polaron always binds, i.e. the energy functional has a minimizer for $N = 1$. Then we discuss the case of multi-polarons containing $N \geq 2$ electrons. We show that their existence is guaranteed when certain quantized binding inequalities of HVZ type are satisfied.

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1. Introduction

A *polaron* is a quantum electron in a polar crystal which is able to form a bound state by using the deformation of the medium which is generated by its own charge [1]. Likewise, a *multi-polaron* or *N -polaron* is the system formed by the interaction of N electrons with a polar crystal.

That a polaron can be in a bound state is a rather simple physical mechanism. When the (negatively charged) electron is added to the medium, it locally repels (respectively attracts) the other electrons (respectively the positively charged nuclei) of the crystal. A local deformation is thus generated in the crystal, and it is itself felt by the added particle. In other words the additional electron carries a “polarization cloud” with it. It is therefore often useful to think of the polaron as a *dressed particle*, that is a single (composite) particle with new physical properties: effective mass, effective charge, etc. For an N -polaron the situation is a bit more involved. Since the effective polarization has to overcome the natural Coulomb repulsion between the particles, bound states do not always exist.

The question of what model to use to describe the polaron is an important and non trivial one. In the Born-Oppenheimer approximation, a quantum crystal is a very complicated object, made of infinitely many nuclei and delocalised electrons. The accurate description of such a system is a very delicate issue and, for this reason, simple effective models are often considered. They should remain mathematically tractable while still capturing as much of the physics of the system as possible.

A famous example is the model of Fröhlich [8, 9] dating back from 1937, in which the crystal is described as an homogeneous quantized polarization field with which the electrons interact. In the limit of strong coupling between the electrons and the field, the model reduces to Pekar’s theory [21, 22, 23, 17, 20]. There the crystal is a classical continuous polarizable model, leading to an effective attractive Coulomb interaction in the energy functional of the theory:

$$\mathcal{E}_{\varepsilon_M}^P[\psi] = \frac{1}{2} \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx + \frac{(\varepsilon_M)^{-1} - 1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi(x)|^2 |\psi(y)|^2}{|x - y|} dx dy. \quad (1.1)$$

Here ψ is the wave-function of the electron, ε_M is the static dielectric constant of the crystal and we work in atomic units. The variational equation corresponding to (1.1) is sometimes called the *Schrödinger-Newton* or *Choquard* equation.

It is the attractive Coulomb term in (1.1) that leads to the existence of bound states of electrons, i.e. minimizers (or ground states) of the energy functional. Whereas the energy functional for electrons in vacuum has no minimizer, Lieb [15] proved the existence and uniqueness (up to translations) of a ground state for Pekar’s functional (1.1).

The same nonlinear attractive term is obtained in Pekar’s model for the N -polaron. Then, as we have already mentioned, depending on the strength of the attractive Coulomb term as compared to the natural repulsion between the electrons, one can get binding or not. It is an important issue to determine in which parameter range binding occurs [10, 6, 7, 13].

The approximations made in the construction of Fröhlich’s and Pekar’s models reduce their applicability to situations where the N -polaron is spread over a region of space much larger than the characteristic size of the underlying crystal. One then speaks of *large polarons*. In [14] we have introduced a new polaron model by coupling the energy functional for electrons in the vacuum to a microscopic model of quantum crystals with defects introduced in [2, 3]. Unlike in Fröhlich and Pekar theories we take the crystal explicitly into account and make no assumption on the size of the electron. Our approach thus qualifies for the description of both small and large polarons. The model takes the following form (for one electron):

$$\mathcal{E}_{\text{eff}}[\psi] = \frac{1}{2} \int_{\mathbb{R}^3} |\nabla \psi(x)|^2 dx + \int_{\mathbb{R}^3} V_{\text{per}}^0(x) |\psi(x)|^2 dx + F_{\text{crys}}[|\psi|^2]. \quad (1.2)$$

Here V_{per}^0 is the (periodic) electric potential generated by the unperturbed crystal, which is felt by any particle added to the system. The nonlinear effective energy F_{crys} represents the interaction energy between the electrons and the crystal. It is defined using a Hartree-Fock theory for the response of the electrons of the crystal to a charge defect. The state of the Fermi sea of the perturbed crystal is given by a one-body density matrix γ , that is a non-negative self-adjoint operator on $L^2(\mathbb{R}^3)$. As in [2, 3], we write

$$\gamma = \gamma_{\text{per}}^0 + Q \quad (1.3)$$

where γ_{per}^0 is the density matrix of the periodic unperturbed crystal and Q is the local deformation induced by the charge defect $|\psi|^2$. The effective energy F_{crys} then takes the form

$$F_{\text{crys}}[|\psi|^2] = \inf_{-\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0} \left(\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_Q(x) |\psi(y)|^2}{|x - y|} dx dy + \mathcal{F}_{\text{crys}}[Q] \right). \quad (1.4)$$

Three main ingredients enter in (1.4):

- Electrons are fermions and must thus satisfy the Pauli exclusion principle, which gives in the formalism of density matrices the constraint $0 \leq \gamma \leq 1$ as operators. This justifies the constraint on admissible perturbations Q imposed in (1.4).
- The electrons forming the polaron interact with the perturbation they induce in the Fermi sea. This is taken into account by the first term in (1.4) where ρ_Q is the charge density associated with Q , given formally by $\rho_Q(x) = Q(x, x)$ (we use the same notation for the operator Q and its kernel).
- Generating a deformation of the Fermi sea has an energetic cost, represented by the functional $\mathcal{F}_{\text{crys}}$ in (1.4). The somewhat complicated definition of this functional will be recalled below. It was derived in [2].

More details on how we arrived at the form above can be found in the introduction of [14]. Let us mention that this model only takes into account the displacement of the electrons of the crystal and neglects that of the nuclei. This is arguably an important restriction, but our model already captures important physical properties of the polaron, and on the other hand this is all we can treat from a mathematical point of view at present.

In this paper we will show that a (single) polaron described by the energy functional (1.4) always binds. The case of N -polarons is more sophisticated, as now the effective attraction resulting from the polarization of the crystal has to overcome the electronic repulsion. The energy functional corresponding to (1.2) in the case of the N -polaron is given by

$$\begin{aligned} \mathcal{E}_{\text{eff}}[\Psi] = \int_{\mathbb{R}^{3N}} \left(\frac{1}{2} \sum_{j=1}^N |\nabla_{x_j} \Psi(x_1, \dots, x_N)|^2 + \sum_{1 \leq k < \ell \leq N} \frac{|\Psi(x_1, \dots, x_N)|^2}{|x_k - x_\ell|} \right) dx_1 \cdots dx_N \\ + \int_{\mathbb{R}^3} V_{\text{per}}^0 \rho_\Psi + F_{\text{crys}}[\rho_\Psi] \end{aligned} \quad (1.5)$$

where ρ_Ψ is the usual density of charge associated with the many-body wavefunction Ψ whose definition is recalled in (2.16) below.

In fact, our model (1.2) is closely related to Pekar's functional. We proved in [14] that Pekar's theory can be recovered from (1.2) in a macroscopic limit where the characteristic size of the underlying crystal goes to 0. In addition to clarifying the physics entering the Pekar model, this result also gives some interesting insight on the model (1.2), in particular, regarding the question of the existence of binding. Indeed, it is known [13] that Pekar's functional has a ground state in some range of parameters. We deduce in [14] that sequences of approximate minimizers for (1.5) converge in the macroscopic limit to a ground state of the Pekar functional, thus showing that our model at least accounts for the binding of large polarons in this regime. In this paper, we want to derive conditions ensuring that there is binding in the case of small polarons where the macroscopic limit argument and the link to Pekar's theory are irrelevant.

Quite generally, for many-body quantum systems, the existence of bound states of N particles depends on the validity of so-called *binding inequalities*. If $E(N)$ denotes the infimum energy of some physical system containing N particles, a ground state containing N particles exists when

$$E(N) < \min_{k=1 \dots N} E(N - k) + E^\infty(k) \quad (1.6)$$

where $E^\infty(N)$ denotes the energy of the same N particle system, but with all particles ‘sent to infinity’. For example, for atoms or molecules comprising N electrons, $E(N)$ includes the contribution of the electric potential generated by the fixed nuclei, while $E^\infty(N)$ does not. Particles ‘at infinity’ no longer see the attraction of the nuclei. Note the formal similarity between inequalities (1.6) and those appearing in Lions’ concentration compactness principle [18, 19], an important mathematical tool used in nonlinear analysis. The major difference is that the former are quantized and thus more difficult to relate to one another. See [13] for a more precise discussion of this connection.

It is not difficult to discuss on physical grounds why inequalities (1.6) are sufficient for the existence of bound states. Indeed, (1.6) says that sending particles to infinity is not favorable from an energetic point of view. In mathematical terms, the inequalities (1.6) avoid the *lack of compactness at infinity* of minimizing sequences. The existence of a ground state then follows from the *local compactness* of the model under consideration. Nevertheless, the mathematical proof that inequalities of the type (1.6) are sufficient for the existence of bound states of N -particles is highly non-trivial because the problems $E(N)$, $E(N - k)$ and $E^\infty(k)$ are set in different Hilbert spaces. In the case of atoms and molecules, the fact that inequalities of the form (1.6) imply the existence of bound states is the content of the famous HVZ theorem, first proved independently in [12, 26, 27].

In this paper we prove an HVZ-type theorem for our polaron functional (1.5) when $N \geq 2$. We have to face two difficulties. First the functional is invariant under the action of arbitrarily large translations (those leaving invariant the periodic lattice of the crystal), so the energy functional does not change when particles are sent to infinity. The correct binding inequalities therefore take the form

$$E(N) < \min_{k=1 \dots N-1} E(N - k) + E(k). \quad (1.7)$$

Second, the energy contains the highly nonlinear term $F_{\text{crys}}[\rho_\Psi]$. We are thus faced with the combination of the difficulties associated with many-body theory and those inherent to nonlinear problems. A general technique has been introduced in [13] to tackle these questions. Our purpose in this paper is to explain how one can deal with the model (1.5) using the method of [13]. Our main task will be to control the behavior of the (highly nonlinear) effective polarization energy F_{crys} .

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2. Statement of the main results

2.1. The mean-field crystal

We begin by recalling the precise definition of the crystal functional entering in (1.2). More details can be found in [2, 3, 14].

We fix an \mathcal{L} -periodic density of charge μ_{per}^0 for the classical nuclei of the crystal, with \mathcal{L} a discrete subgroup of \mathbb{R}^3 . It is enough for our purpose to assume that μ_{per}^0 is a locally-finite non-negative measure, such that $\int_\Gamma \mu_{\text{per}}^0 = Z \in \mathbb{N}$, where $\Gamma = \mathbb{R}^3/\mathcal{L}$ is the unit cell.

In reduced Hartree-Fock theory, the state of the electrons in the crystal is described by a *one-particle density matrix*, which is a self-adjoint operator $\gamma : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ such that $0 \leq \gamma \leq 1$ (in the sense of operators). When no external field is applied to the system, the electrons arrange

in a periodic configuration $\gamma = \gamma_{\text{per}}^0$, which is a solution of the *reduced Hartree-Fock equations*¹

$$\begin{cases} \gamma_{\text{per}}^0 = \mathbb{1}_{(-\infty, \varepsilon_F)}(-\Delta/2 + V_{\text{per}}^0), \\ -\Delta V_{\text{per}}^0 = 4\pi(\rho_{\gamma_{\text{per}}^0} - \mu_{\text{per}}^0), \\ \int_{\Gamma} \rho_{\gamma_{\text{per}}^0} = \int_{\Gamma} \mu_{\text{per}}^0 = Z. \end{cases} \quad (2.1)$$

Here ρ_A denotes the density of the operator A which is formally given by $\rho_A(x) = A(x, x)$ when A is locally trace-class. Also, $\mathbb{1}_{(-\infty, \varepsilon_F)}(H)$ denotes the spectral projector of H onto the interval $(-\infty, \varepsilon_F)$. The real number ε_F in (2.1) is called the *Fermi level*. It is also the Lagrange multiplier used to impose the constraint that the system must be locally neutral (third equation in (2.1)). The unique solution to the self-consistent equation (2.1) is found by minimizing the so-called reduced Hartree-Fock energy functional [5, 2].

We are working in the so-called atomic units in which the mass m and the charge e of the electrons of the crystal are set to $m = e = 1$. Also we neglect their spin for simplicity (reinserting the spin in our model is straightforward).

By Bloch-Floquet theory [24], the spectrum of the \mathcal{L} -periodic Schrödinger operator

$$H_{\text{per}}^0 = -\frac{1}{2}\Delta + V_{\text{per}}^0(x)$$

is composed of bands. When there is a gap between the Z th and the $(Z+1)$ st bands, the crystal is an insulator and ε_F can be any arbitrary number in the gap. As in [2], in the whole paper we will assume that the host crystal is an insulator.

Asumption 2.1 (The host crystal is an insulator).

The periodic Schrödinger operator H_{per}^0 has a gap between its Z th and $(Z+1)$ st bands, and we fix any chemical potential ε_F in the corresponding gap.

When the quantum crystal is submitted to an external field, the Fermi sea polarizes. The method used in [2] to define the energetic cost of such a polarization relies on the following idea. The energetic cost to move the electrons from γ_{per}^0 to γ is defined as the (formal) difference between the (infinite) reduced Hartree-Fock energies of γ and of γ_{per}^0 . Denoting by

$$D(f, g) := \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)f(y)}{|x-y|} dx dy = 4\pi \int_{\mathbb{R}^3} \frac{\overline{\hat{f}(k)}\hat{g}(k)}{|k|^2} dk \quad (2.2)$$

the Coulomb interaction (where \hat{f} denotes the Fourier transform of f), one arrives at the functional

$$\mathcal{F}_{\text{crys}}[Q] := \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_F)Q) + \frac{1}{2}D(\rho_Q, \rho_Q) \quad (2.3)$$

where Tr_0 denotes a generalized trace, see (2.6) and (2.9) below. For convenience we also denote

$$\mathcal{F}_{\text{crys}}[\rho, Q] := \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_F)Q) + \frac{1}{2}D(\rho_Q, \rho_Q) + D(\rho, \rho_Q). \quad (2.4)$$

The functional setting in which the terms of these equations make sense is defined as follows. Any operator Q satisfying the constraint

$$-\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0 \quad (2.5)$$

is decomposed as

$$Q = Q^{--} + Q^{-+} + Q^{++} + Q^{+-} \quad (2.6)$$

¹Sometimes called *Hartree equations* in the physics literature.

where $Q^{--} = \gamma_{\text{per}}^0 Q \gamma_{\text{per}}^0$, $Q^{-+} = \gamma_{\text{per}}^0 Q (1 - \gamma_{\text{per}}^0)$, and so on. It is proved in [2] that for Q satisfying (2.5) and $\nu \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, $\mathcal{F}_{\text{crys}}[\nu, Q]$ is finite if and only if Q is in the function space

$$\mathcal{Q} = \left\{ Q \in \mathfrak{S}^2 \mid Q = Q^*, |\nabla|Q \in \mathfrak{S}^2, Q^{++}, Q^{--} \in \mathfrak{S}^1, |\nabla|Q^{++}|\nabla|, |\nabla|Q^{--}|\nabla| \in \mathfrak{S}^1 \right\} \quad (2.7)$$

that we equip with its natural norm

$$\|Q\|_{\mathcal{Q}} = \|Q\|_{\mathfrak{S}^2} + \|Q^{++}\|_{\mathfrak{S}^1} + \|Q^{--}\|_{\mathfrak{S}^1} + \| |\nabla|Q \|_{\mathfrak{S}^2} + \| |\nabla|Q^{++}|\nabla| \|_{\mathfrak{S}^1} + \| |\nabla|Q^{--}|\nabla| \|_{\mathfrak{S}^1}. \quad (2.8)$$

The symbols \mathfrak{S}^1 and \mathfrak{S}^2 denote the Schatten classes of trace-class and Hilbert-Schmidt operators on $L^2(\mathbb{R}^3)$ respectively (see [25] and [24]). For operators in \mathcal{Q} , the kinetic energy in (2.3) is defined as

$$\text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Q = \text{Tr} \left(|H_{\text{per}}^0 - \varepsilon_F|^{1/2} (Q^{++} - Q^{--}) |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right), \quad (2.9)$$

see [2]. More generally, one can define the *generalized trace* as

$$\text{Tr}_0 Q = \text{Tr} Q^{++} + \text{Tr} Q^{--} \quad (2.10)$$

when Q^{++} and Q^{--} are trace-class. Note that Tr_0 differs from the usual trace Tr , the operators in \mathcal{Q} not being trace-class in general. They nevertheless have an unambiguously defined density $\rho_Q \in L_{\text{loc}}^1(\mathbb{R}^3)$ (see [2], Proposition 1). It belongs to $L^2(\mathbb{R}^3)$ and to the Coulomb space

$$\mathcal{C} = \left\{ \rho \mid D(\rho, \rho)^{1/2} < \infty \right\} \quad (2.11)$$

and it holds by definition

$$\text{Tr}_0(VQ) = \int_{\mathbb{R}^3} V \rho_Q \quad (2.12)$$

for any $V \in \mathcal{C}'$.

Having defined in (2.3) the total energetic cost to go from γ_{per}^0 to $\gamma_{\text{per}}^0 + Q$, we can give a sense to the energetic response of the crystal to an external density ν . The state of the Fermi sea is obtained by solving the following minimization problem

$$\boxed{F_{\text{crys}}[\nu] = \inf_{-\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0} \left(D(\nu, \rho_Q) + \mathcal{F}_{\text{crys}}[Q] \right)}. \quad (2.13)$$

As shown in [2], for any $\nu \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, this minimization problem has at least one solution in \mathcal{Q} . The corresponding density ρ_Q is in $L^2(\mathbb{R}^3)$ but in general it has long range oscillations which are not integrable at infinity [4].

2.2. The small polaron

To our crystal we now add N quantum particles, which are by assumption distinguishable from those of the crystal. In reality they are electrons having the same mass $m = 1$ as those of the crystal, but we want to keep m arbitrary to emphasize that in our model the additional particles behave differently from those of the crystal. This will also allow us to compare with the results we have obtained in [14].

The total energy of the system now includes the term $F_{\text{crys}}[\nu]$ with $\nu = |\psi|^2$ (polaron) or $\nu = \rho_\Psi$ (N -polaron). For the single polaron, the energy is given by

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^3} \left(\frac{1}{2m} |\nabla \psi(x)|^2 + V_{\text{per}}^0(x) |\psi(x)|^2 \right) dx + F_{\text{crys}}[|\psi|^2]. \quad (2.14)$$

For the N -polaron with $N \geq 2$ it reads

$$\begin{aligned} \mathcal{E}[\Psi] = \int_{\mathbb{R}^{3N}} & \left(\frac{1}{2m} \sum_{j=1}^N |\nabla_{x_j} \Psi(x_1, \dots, x_N)|^2 + \sum_{1 \leq k < \ell \leq N} \frac{|\Psi(x_1, \dots, x_N)|^2}{|x_k - x_\ell|} \right) dx_1 \cdots dx_N \\ & + \int_{\mathbb{R}^3} V_{\text{per}}^0(x) \rho_\Psi(x) dx + F_{\text{crys}}[\rho_\Psi]. \end{aligned} \quad (2.15)$$

As we think that there is no possible confusion, we do not emphasize the particle number N in our notation of the energy \mathcal{E} . The density ρ_Ψ is defined as

$$\rho_\Psi(x) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi(x, x_2, \dots, x_N)|^2 dx_2 \dots dx_N. \quad (2.16)$$

The corresponding ground state energies read

$$E(1) := \inf \left\{ \mathcal{E}[\psi], \psi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\psi|^2 = 1 \right\} \quad (2.17)$$

and

$$E(N) := \inf \left\{ \mathcal{E}[\Psi], \Psi \in H^1(\mathbb{R}^{3N}), \Psi \text{ fermionic}, \int_{\mathbb{R}^{3N}} |\Psi|^2 = 1 \right\}. \quad (2.18)$$

Here by ‘fermionic’ we mean antisymmetric under particle exchange:

$$\Psi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = -\Psi(x_1, \dots, x_j, \dots, x_i, \dots, x_N) \text{ for any } i \neq j \quad (2.19)$$

as is appropriate for electrons. Recall that we have neglected the spin for simplicity.

We now state our main results. In the single polaron case we are able to show the existence of a bound state.

Theorem 2.1 (Existence of small polarons).

For $N = 1$, we have

$$E(1) < E_{\text{per}} := \inf \sigma \left(-\frac{1}{2m} \Delta + V_{\text{per}}^0 \right). \quad (2.20)$$

There are always minimizers for $E(1)$ and all the minimizing sequences converge to a minimizer for $E(1)$ strongly in $H^1(\mathbb{R}^3)$, up to extraction of a subsequence and up to translations.

Inequality (2.20) expresses the fact that binding is energetically favorable : the right-hand side is the energy an electron would have in absence of binding.

In the N -polaron case we can give necessary and sufficient conditions for the compactness of minimizing sequences.

Theorem 2.2 (HVZ for small N -polarons).

For $N \geq 2$, the following assertions are equivalent:

(1) One has

$$E(N) < E(N - k) + E(k) \text{ for all } k = 1, \dots, N - 1. \quad (2.21)$$

(2) Up to translation and extraction of a subsequence, all the minimizing sequences for $E(N)$ converge to a minimizer for $E(N)$ strongly in $H^1(\mathbb{R}^{3N})$.

Remark 2.1. For this result, the fermionic nature of the electrons is not essential. The same theorem holds if the electrons are replaced by bosons, i.e. the wave function Ψ is supposed to be symmetric under particle exchange.

As discussed in the introduction, this theorem is rather natural from a physical point of view. It is not expected that the conditions (2.21) hold in general. As in Pekar’s theory, one should expect the existence of minimizers to depend on the choice of parameters entering the functional (in our case only the periodic distribution μ_{per}^0 of the nuclei). Testing the validity of these inequalities is a challenging task that would require more knowledge on the properties of the crystal model than we presently have. In particular, the decay at infinity of the minimizers of the crystal model should be investigated.

In [14] we have considered a macroscopic limit in which V_{per}^0 is replaced by $m^{-1}V_{\text{per}}^0(x/m)$ and $F_{\text{crys}}[\rho_\Psi]$ is replaced by $m^{-1}F_{\text{crys}}[m^3\rho_\Psi(m\cdot)]$. By scaling, this is actually the same as letting the mass m of the polarons tend to zero in the model considered in this article. In the limit $m \rightarrow 0$

the ground state energy $E_m(N)$ converges to Pekar's energy involving the macroscopic dielectric constant ε_M of the crystal defined in [4] (up to a simple oscillatory factor, see [14] for details). It was shown in [13] that the binding inequalities are satisfied in Pekar's theory when ε_M is large enough. We conclude that in this case they will also be satisfied for m small enough and therefore minimizers do exist in this case.

The rest of the paper is devoted to the proof of Theorem 2.2. One of us has considered in Section 5 of [13] a general class of nonlinear many-body problems of the form

$$\int_{\mathbb{R}^{3N}} \left(\frac{1}{2} \sum_{j=1}^N |\nabla_{x_j} \Psi(x_1, \dots, x_N)|^2 + \sum_{1 \leq k < \ell \leq N} |\Psi(x_1, \dots, x_N)|^2 W(x_k - x_\ell) \right) dx_1 \cdots dx_N + F[\rho\Psi]$$

and provided sufficient assumptions on the interaction potential W and the non linearity F under which a HVZ type result similar to Theorem 2.2 holds. The assumptions on W include the Coulomb interaction we are concerned with in this paper but, unfortunately, our crystal functional F_{crys} does not seem to satisfy all the properties imposed on F in [13]. Also the presence of the periodic potential V_{per}^0 adds a new difficulty. Nevertheless the general strategy of [13] still applies and our goal in this paper is to explain how to overcome the difficulties associated with F_{crys} .

Section 3 gathers some important properties of the crystal functional that are to be used in the proofs of Theorems 2.1 and 2.2, presented in Sections 4 and 5 respectively.

3. Properties of the crystal energy

In this section we roughly speaking prove that F_{crys} satisfies Assumptions (A1) to (A5) of [13], Section 5. We are only able to prove a little less, but the properties we do prove are sufficient for the proof of Theorem 2.2 as we explain in Section 5.

We start in Section 3.1 with almost immediate consequences of the definition of F_{crys} , and devote Section 3.3 to the more involved fact that our crystal functional satisfies a 'decoupling at infinity' property. The proof of this property requires some facts about localization operators that we gather in Section 3.2.

3.1. Concavity, subcriticality and translation invariance

The following is the equivalent of Assumptions (A4) and (A5) in [13], Section 5.

Lemma 3.1 (Concavity).

F_{crys} is concave on $\{\rho \in \mathcal{C}, \rho \geq 0\}$. Moreover it is strictly concave at the origin:

$$F_{\text{crys}}[t\rho] > tF_{\text{crys}}[\rho] \quad (3.1)$$

for all $\rho \in \mathcal{C}$, $\rho \geq 0$ and all $0 < t < 1$.

Proof. The functional $\mathcal{F}_{\text{crys}}[\rho, Q]$ defined in (2.4) is linear in ρ . As by definition

$$F_{\text{crys}}[\rho] = \inf \{ \mathcal{F}_{\text{crys}}[\rho, Q], -\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0 \},$$

it is clearly a concave functional of ρ . As for the strict concavity we note that

$$\mathcal{F}_{\text{crys}}[t\rho, Q] = \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_F)Q) + \frac{1}{2}D(\rho_Q, \rho_Q) + tD(\rho, \rho_Q) > t\mathcal{F}_{\text{crys}}[\rho, Q] \geq tF_{\text{crys}}[\rho]$$

for all $0 < t < 1$ by positivity of the kinetic and Coulomb energies. Taking for Q the minimizer corresponding to $t\rho$ which is known to exist by [2, 4] proves (3.1). \square

The next lemma will be useful to prove that minimizing sequences for our polaron model are bounded in $H^1(\mathbb{R}^{3N})$. It is the equivalent of Assumption (A3) in [13], Section 5.

Lemma 3.2 (Subcriticality).

The functional F_{crys} is locally uniformly continuous on $L^{6/5}$. More precisely, we have

$$|F_{\text{crys}}[\rho] - F_{\text{crys}}[\rho']| \leq C \|\rho - \rho'\|_{L^{6/5}}^2 \quad (3.2)$$

for a universal constant $C > 0$. Moreover, for every $\varepsilon > 0$, we have

$$0 > F_{\text{crys}}[|\varphi|^2] \geq -\varepsilon \int_{\mathbb{R}^3} |\nabla \varphi|^2 - \frac{C}{\varepsilon} \left(\int_{\mathbb{R}^3} |\varphi|^2 \right)^3 \quad (3.3)$$

for all $\varphi \in H^1(\mathbb{R}^3)$.

Proof. For any $\rho \in L^{6/5}$ and any $Q \in Q$ we can complete the square in the electrostatic terms of $\mathcal{F}_{\text{crys}}[\rho, Q]$ and obtain

$$\mathcal{F}_{\text{crys}}[\rho, Q] = \text{Tr}_0 \left((H_{\text{per}}^0 - \varepsilon_F) Q \right) + \frac{1}{2} D(\rho_Q + \rho, \rho_Q + \rho) - \frac{1}{2} D(\rho, \rho) \geq -\frac{1}{2} D(\rho, \rho).$$

Taking the infimum with respect to Q and applying this with $\rho = |\varphi|^2$ immediately yields

$$F_{\text{crys}}[|\varphi|^2] \geq -\frac{1}{2} D(|\varphi|^2, |\varphi|^2) \geq -C \|\varphi\|_{L^{12/5}}^4$$

by the Hardy-Littlewood-Sobolev inequality ([16], Theorem 4.3). Using now the Sobolev and Hölder inequalities we get as stated

$$\|\varphi\|_{L^{12/5}}^4 \leq \|\varphi\|_{L^6} \|\varphi\|_{L^2}^3 \leq \varepsilon \int_{\mathbb{R}^3} |\nabla \varphi|^2 + \frac{C}{\varepsilon} \left(\int_{\mathbb{R}^3} |\varphi|^2 \right)^3.$$

Then, replacing ρ by $\rho - \rho'$ we also have

$$\mathcal{F}_{\text{crys}}[\rho - \rho', Q] \geq -\frac{1}{2} D(\rho - \rho', \rho - \rho').$$

Choosing now for Q a minimizer of $\mathcal{F}_{\text{crys}}[\rho, Q]$ we deduce

$$F_{\text{crys}}[\rho] - F_{\text{crys}}[\rho'] \geq -\frac{1}{2} D(\rho - \rho', \rho - \rho').$$

Without loss of generality we can assume that the left-hand side is negative. We conclude that there exists a constant such that

$$|F_{\text{crys}}[\rho] - F_{\text{crys}}[\rho']| \leq C \|\rho - \rho'\|_{L^{6/5}}^2$$

using the Hardy-Littlewood-Sobolev inequality again. \square

Finally, we note that our functional is invariant under the action of the translations of the periodic lattice \mathcal{L} . Note that in [13], full translation invariance is assumed (see Assumption (A2)). However, what is really used in the proof of the results there is the invariance under the action of arbitrarily large translations.

Lemma 3.3 (Translation invariance).

For any $\rho \in L^{6/5}$ and any translation $\vec{\tau} \in \mathcal{L}$ of the periodic lattice,

$$F_{\text{crys}}[\rho(\cdot + \vec{\tau})] = F_{\text{crys}}[\rho]. \quad (3.4)$$

Proof. We denote by Q a minimizer of $\mathcal{F}_{\text{crys}}[\rho, Q]$. Clearly $\rho_Q(\cdot + \vec{\tau}) = \rho_{U_{\vec{\tau}}^* Q U_{\vec{\tau}}}$ where $U_{\vec{\tau}}$ is the unitary translation operator acting on $L^2(\mathbb{R}^3)$ and defined by $U_{\vec{\tau}} f = f(\cdot - \vec{\tau})$. We deduce

$$F_{\text{crys}}[\rho(\cdot + \vec{\tau})] \leq \mathcal{F}_{\text{crys}}[\rho(\cdot + \vec{\tau}), \vec{\tau}^* Q \vec{\tau}] = \text{Tr}_0 \left(\vec{\tau} (H_{\text{per}}^0 - \varepsilon_F) \vec{\tau}^* Q \right) + \frac{1}{2} D(\rho, \rho_Q) - D(\rho, \rho_Q) = F_{\text{crys}}[\rho]$$

by translation invariance of the Coulomb interaction and the fact that H_{per}^0 commutes with the translations of the lattice \mathcal{L} . Exchanging the roles of $\rho(\cdot + \vec{\tau})$ and ρ and applying the same argument proves that there must be equality. \square

3.2. Some localization properties

In order to prove that the crystal energy of two distant clusters of mass decouples we will use a localization procedure. We here provide several facts about this procedure that will be useful in the next section.

We will use the following local compactness criterion in Schatten classes. Its standard proof is omitted.

Lemma 3.4 (Local compactness in Schatten spaces).

Denote by \mathfrak{S}^p the class of compact operators A of some Hilbert space \mathfrak{h} such that $(\text{Tr}(|A|^p))^{1/p} < +\infty$, with the convention that \mathfrak{S}^∞ denotes the class of compact operators.

- If $A_n \rightharpoonup A$ weakly- $*$ in \mathfrak{S}^1 and $K, K' \in \mathfrak{S}^\infty$ then $KA_nK' \rightarrow KAK'$ strongly in \mathfrak{S}^1 .
- If $A_n \rightharpoonup A$ weakly in \mathfrak{S}^r , $K \in \mathfrak{S}^p$ and $K' \in \mathfrak{S}^q$ then $KA_nK' \rightarrow KAK'$ strongly in \mathfrak{S}^s with $1/s = 1/p + 1/q + 1/r$.

We next prove an interesting property concerning the localization of functions of the Coulomb space \mathcal{C} .

Lemma 3.5 (Localization in the Coulomb space \mathcal{C}).

Let $\chi \in L^\infty(\mathbb{R}^3)$ be such that $\nabla\chi \in L^3(\mathbb{R}^3)$. Then $\chi\rho \in \mathcal{C}$ for all $\rho \in \mathcal{C}$. More precisely, there exists a universal constant $C > 0$ such that

$$\|\chi\rho\|_{\mathcal{C}} \leq C (\|\chi\|_{L^\infty} + \|\nabla\chi\|_{L^3}) \|\rho\|_{\mathcal{C}}. \quad (3.5)$$

Proof. Recall that \mathcal{C} is the dual of the homogeneous Sobolev space $\dot{H}^1(\mathbb{R}^3)$. For any $V \in C_c^\infty(\mathbb{R}^3)$ we have by the Sobolev inequality

$$\begin{aligned} \left| \int_{\mathbb{R}^3} \chi\rho V \right| &\leq (4\pi)^{-1/2} \|\rho\|_{\mathcal{C}} \|\nabla(\chi V)\|_{L^2} \\ &\leq (4\pi)^{-1/2} \|\rho\|_{\mathcal{C}} \left(\|\chi\|_{L^\infty} \|\nabla V\|_{L^2} + \|\nabla\chi\|_{L^3} \|V\|_{L^6} \right) \\ &\leq (4\pi)^{-1/2} \|\rho\|_{\mathcal{C}} \left(\|\chi\|_{L^\infty} + C \|\nabla\chi\|_{L^3} \right) \|\nabla V\|_{L^2} \end{aligned}$$

and the result follows. \square

Note that for a typical smooth localization function χ_R^2 defined by $\chi_R(x) = \chi(x/R)$ with $\chi \equiv 1$ in $B(0, R)$, $\chi \equiv 0$ in $B(0, 2)$, the right-hand side of (3.5) does not depend on R :

$$\|\nabla(\chi_R^2)\|_{L^3}^3 = 2^3 \int_{\mathbb{R}^3} \chi_R^3 |\nabla\chi_R|^3 = 2^3 R^{-3} \int_{\mathbb{R}^3} \chi(x/R)^3 |\nabla\chi(x/R)|^3 dx = 2^3 \int_{\mathbb{R}^3} \chi^3 |\nabla\chi|^3 \quad (3.6)$$

This is what makes the lemma particularly useful. For such a localization function we also have the following approximation result:

Lemma 3.6 (Approximation in the Coulomb space).

For any $\rho \in \mathcal{C}$, we have $(\chi_R)^2 \rho \rightarrow \rho$ strongly in \mathcal{C} .

Proof. Recall that $\|\chi_R^2 \rho\|_{\mathcal{C}} \leq C \|\rho\|_{\mathcal{C}}$ with a constant C that is independent of R , by (3.6) and Lemma 3.5. So we can use an “ $\varepsilon/2$ argument”, and replace ρ by a function $\rho' \in L^{6/5}$, for which the statement follows from the Hardy-Littlewood-Sobolev inequality. \square

It will be important in the sequel to know that weak convergence of a sequence (Q_n) in \mathcal{Q} implies strong local compactness of the corresponding ρ_{Q_n} :

Lemma 3.7 (Local compactness for charge densities).

Let (Q_n) be a bounded sequence in \mathcal{Q} such that $Q_n \rightharpoonup Q$ weakly in \mathcal{Q} . Then $\rho_{Q_n} \rightharpoonup \rho_Q$ weakly in $L^2 \cap \mathcal{C}$ and strongly in L^1_{loc} .

Proof. We know from Proposition 1 in [2] that $\rho_{Q_n} \rightharpoonup \rho_Q$ weakly in $L^2 \cap \mathcal{C}$. Only the strong local convergence is new. The latter follows from the statement that

$$\chi Q_n \chi \rightarrow \chi Q \chi$$

strongly in the trace-class \mathfrak{S}^1 , for every smooth function χ of compact support. To see this, we write as usual

$$Q_n = Q_n^{++} + Q_n^{-+} + Q_n^{+-} + Q_n^{--} \quad (3.7)$$

and consider only the first two terms as the other two can be dealt with in a similar way. We have

$$\chi Q_n^{++} \chi = \left\{ \chi (-\Delta + 1)^{-1/2} \right\} \left\{ (-\Delta + 1)^{1/2} Q_n^{++} (-\Delta + 1)^{1/2} \right\} \left\{ (-\Delta + 1)^{-1/2} \chi \right\}.$$

The operator $\chi (-\Delta + 1)^{-1/2}$ is compact and $(-\Delta + 1)^{1/2} Q_n^{++} (-\Delta + 1)^{1/2}$ converges towards $(-\Delta + 1)^{1/2} Q^{++} (-\Delta + 1)^{1/2}$ weakly-* in \mathfrak{S}^1 by assumption. By Lemma 3.4 we deduce that $\chi Q_n^{++} \chi \rightarrow \chi Q^{++} \chi$ strongly in \mathfrak{S}^1 .

We argue similarly for the off diagonal terms, writing this time

$$\chi Q_n^{+-} \chi = \left\{ \chi (-\Delta + 1)^{-1/2} \right\} \left\{ (-\Delta + 1)^{1/2} Q_n^{+-} \right\} \left\{ \gamma_{\text{per}}^0 \chi \right\}.$$

Again the operator $\chi (-\Delta + 1)^{-1/2}$ is compact and we can write

$$\gamma_{\text{per}}^0 \chi = \gamma_{\text{per}}^0 (H_{\text{per}}^0 + \mu) (H_{\text{per}}^0 + \mu)^{-1} (1 - \Delta) (1 - \Delta)^{-1} \chi.$$

Here μ is a large enough constant such that $H_{\text{per}}^0 \geq -\mu/2$. The operator $\gamma_{\text{per}}^0 (H_{\text{per}}^0 + \mu)$ is bounded by the functional calculus. Also, $(H_{\text{per}}^0 + \mu)^{-1} (1 - \Delta)$ is bounded by Lemma 1 in [2]. Finally, $(1 - \Delta)^{-1} \chi \in \mathfrak{S}^2$. Thus $\gamma_{\text{per}}^0 \chi \in \mathfrak{S}^2$. Since $(-\Delta + 1)^{1/2} Q_n^{+-} \rightharpoonup (-\Delta + 1)^{1/2} Q^{+-}$ weakly in \mathfrak{S}^2 by assumption, we deduce by Lemma 3.4 again, that $\chi Q_n^{+-} \chi \rightarrow \chi Q^{+-} \chi$ strongly in \mathfrak{S}^1 .

We have proved that $\chi Q_n \chi \rightarrow \chi Q \chi$ strongly in \mathfrak{S}^1 , but $\rho_{\chi Q_n \chi} = \chi^2 \rho_{Q_n}$, so we deduce that $\rho_{Q_n} \rightarrow \rho_Q$ strongly in L_{loc}^1 . \square

Finally, the following algebraic property, which does not seem to have been noticed before, will be very useful when constructing trial states for the crystal functional.

Lemma 3.8 (Adding states using localization).

Let Π be an orthogonal projector on a Hilbert space \mathfrak{H} , and χ, η two self-adjoint operators on \mathfrak{H} such that $\chi^2 + \eta^2 \leq 1$. We introduce the corresponding localization operators

$$X = \Pi \chi \Pi + (1 - \Pi) \chi (1 - \Pi) \quad \text{and} \quad Y = \Pi \eta \Pi + (1 - \Pi) \eta (1 - \Pi).$$

Let Q, Q' two self-adjoint operators such that $-\Pi \leq Q, Q' \leq 1 - \Pi$. Then we have

$$-\Pi \leq X Q X + Y Q' Y \leq 1 - \Pi \quad (3.8)$$

as well.

Proof. We have $-X \Pi X - Y \Pi Y \leq X Q X + Y Q' Y \leq X(1 - \Pi)X + Y(1 - \Pi)Y$. Now, the result follows from the estimate

$$X \Pi X + Y \Pi Y = \Pi \chi \Pi \chi \Pi + \Pi \eta \Pi \eta \Pi \leq \Pi (\chi^2 + \eta^2) \Pi \leq \Pi$$

and the equivalent one Π replaced by $1 - \Pi$. \square

Typically, one can think of χ and η as being two localization functions satisfying $\chi^2 + \eta^2 = 1$. In our context, the projector Π will be γ_{per}^0 and the main virtue of the corresponding operators X and Y is that they commute with γ_{per}^0 .

3.3. Decoupling at infinity

Here we provide the most crucial ingredient of the proof of Theorem 2.2, namely the fact that the crystal energy of the sum of two distant pieces of mass is almost the sum of the energies of these pieces. This is the content of the following proposition, which is the equivalent of assumption (A3) in [13]. Note however that we prove much less than what is stated there. Fortunately, the proof of Theorem 25 in [13] does not actually require such a strong assumption as (A3), as we will show in Section 5 below.

Proposition 3.1 (Decoupling at infinity).

Let (ρ_n) be a bounded sequence in the Coulomb space \mathcal{C} such that $\rho_n \rightharpoonup \rho$ weakly. Then

$$\lim_{n \rightarrow \infty} \left(F_{\text{crys}}[\rho_n] - F_{\text{crys}}[\rho] - F_{\text{crys}}[\rho_n - \rho] \right) = 0. \quad (3.9)$$

In the above, one should think of ρ_n as being constituted of two clusters of mass, ρ and $\rho_n - \rho$, whose “supports” are infinitely far away in the limit $n \rightarrow \infty$. This is mathematically materialized by the weak convergence to 0 of $\rho_n - \rho$. The proposition then says that the total energy is the sum of the energy of the pieces, up to a small error. Proving (3.9) is a difficult task because of the long range behavior of the response of the crystal : it is known [4] that the polarization ρ_Q of the Fermi sea has long range oscillations that are not integrable at infinity. The oscillations generated by ρ are seen by $\rho_n - \rho$ (and conversely) but, fortunately, they contribute a small amount to the total energy, which is controlled by the Coulomb norm and not the L^1 norm.

Assumption (A3) in [13] is a little different from (3.9). There it was assumed that $\rho_n = \rho_n^1 + \rho_n^2$ where ρ_n^1 and ρ_n^2 are bounded in $L^{6/5}$ and that the distance between their supports goes to infinity, with no assumption on the size of these supports. In Proposition 3.1 it is implicit that one of the two clusters of mass has a support of bounded size and is approximated by its weak limit ρ . This additional assumption is harmless for our purpose because we are dealing with a locally compact problem.

In the course of the proof of Proposition 3.1 we will establish the following, which we believe is of independent interest. It gives the weak continuity of the (multi-valued) map $\rho_n \mapsto Q_n = \operatorname{argmin} \mathcal{F}_{\text{crys}}[\rho_n, \cdot]$.

Corollary 3.1 (A weak continuity result for $\mathcal{F}_{\text{crys}}$).

Let (ρ_n) be a bounded sequence in the Coulomb space \mathcal{C} such that $\rho_n \rightharpoonup \rho$ weakly and Q_n be any minimizer of $\mathcal{F}_{\text{crys}}[\rho_n, \cdot]$. Then, up to extraction of a subsequence, $Q_n \rightharpoonup Q$ weakly in \mathcal{Q} where Q minimizes $\mathcal{F}_{\text{crys}}[\rho, \cdot]$.

We now present the

Proof of Proposition 3.1. We begin with the more difficult part, that is the proof of the lower bound corresponding to (3.9):

Step 1: Lower bound. We denote by Q_n a minimizer for $Q \mapsto \mathcal{F}_{\text{crys}}[\rho_n, Q]$. Corollary 2 in [2] states that the energy functional $\mathcal{F}_{\text{crys}}[\rho_n, Q]$ controls the norm $\|Q\|_{\mathcal{Q}}$:

$$0 \geq \mathcal{F}_{\text{crys}}[\rho_n, Q_n] \geq C \|Q_n\|_{\mathcal{Q}} - \frac{1}{2} D(\rho_n, \rho_n).$$

The upper bound is obtained by taking a trial state $Q \equiv 0$. Using that ρ_n is bounded in \mathcal{C} , hence that $D(\rho_n, \rho_n)$ is bounded, we deduce that the sequence (Q_n) is bounded in \mathcal{Q} . Up to extraction of a subsequence, we can assume that $Q_n \rightharpoonup Q$ and, by Lemma 3.7, that $\rho_{Q_n} \rightharpoonup \rho_Q$ weakly in $L^2 \cap \mathcal{C}$ and strongly in L^1_{loc} .

We now introduce a smooth partition of unity $\chi^2 + \eta^2 = 1$ such that $\chi \equiv 1$ on the ball $B(0, 1)$ and $\chi \equiv 0$ outside of the ball $B(0, 2)$. Similarly, $\eta \equiv 1$ on $\mathbb{R}^3 \setminus B(0, 2)$ and $\eta \equiv 0$ on $B(0, 1)$. We also assume that $\nabla \chi$ and $\nabla \eta$ are bounded functions. Then we introduce $\chi_R(x) := \chi(x/R)$ and

$\eta_R(x) = \eta(x/R)$. In our proof R is fixed and will go to infinity only in the end, after we have taken the limit $n \rightarrow \infty$. Since

$$\|\nabla(\eta_R)^2\|_{L^3}^3 = \|\nabla(\chi_R)^2\|_{L^3}^3 = 2^3 R^{-3} \int_{\mathbb{R}^3} \chi(x/R)^3 |\nabla \chi(x/R)|^3 dx = 2^3 \int_{\mathbb{R}^3} \chi^3 |\nabla \chi|^3$$

is independent of R and $\|\chi_R\|_{L^\infty} \leq 1$ and $\|\eta_R\|_{L^\infty} \leq 1$ by definition, we conclude that

$$\|\rho_{Q_n} \eta_R^2\|_{\mathcal{C}} + \|\rho_{Q_n} \chi_R^2\|_{\mathcal{C}} \leq C \quad (3.10)$$

uniformly in n and R , by Lemma 3.5. Also, $(\chi_R)^2 \rho_{Q_n} \rightarrow (\chi_R)^2 \rho_Q$ strongly in L^1 and weakly in L^2 , thus also strongly in $L^{6/5}$ by interpolation. In particular, $(\chi_R)^2 \rho_{Q_n} \rightarrow (\chi_R)^2 \rho_Q$ strongly in \mathcal{C} by the Hardy-Littlewood-Sobolev inequality.

We start by writing

$$D(\rho_{Q_n}, \rho_n) = D(\rho_{Q_n}, \rho) + D((\eta_R)^2 \rho_{Q_n}, \rho_n - \rho) + D((\chi_R)^2 \rho_{Q_n}, \rho_n - \rho).$$

Note first that

$$\lim_{n \rightarrow \infty} D(\rho_{Q_n}, \rho) = D(\rho_Q, \rho) \quad \text{and} \quad \lim_{n \rightarrow \infty} D((\chi_R)^2 \rho_{Q_n}, \rho_n - \rho) = 0$$

since $\rho_n - \rho \rightarrow 0$ weakly in \mathcal{C} and $(\chi_R)^2 \rho_{Q_n} \rightarrow (\chi_R)^2 \rho_Q$ strongly in \mathcal{C} . So we conclude that

$$\lim_{n \rightarrow \infty} \left(D(\rho_{Q_n}, \rho_n) - D(\rho_Q, \rho) - D((\eta_R)^2 \rho_{Q_n}, \rho_n - \rho) \right) = 0.$$

Then we write in a similar fashion

$$D(\rho_{Q_n}, \rho_{Q_n}) = D((\chi_R)^2 \rho_{Q_n}, (\chi_R)^2 \rho_{Q_n}) + 2D((\chi_R)^2 \rho_{Q_n}, (\eta_R)^2 \rho_{Q_n}) + D((\eta_R)^2 \rho_{Q_n}, (\eta_R)^2 \rho_{Q_n})$$

and conclude that

$$\lim_{n \rightarrow \infty} \left(D(\rho_{Q_n}, \rho_{Q_n}) - D((\chi_R)^2 \rho_Q, (\chi_R)^2 \rho_Q) - 2D((\chi_R)^2 \rho_Q, (\eta_R)^2 \rho_Q) - D((\eta_R)^2 \rho_{Q_n}, (\eta_R)^2 \rho_{Q_n}) \right) = 0.$$

Following ideas from [11, 2], we now consider a better localization method for Q_n which respects the constraint (2.5). We define the two localization operators

$$\begin{aligned} X_R &= \gamma_{\text{per}}^0 \chi_R \gamma_{\text{per}}^0 + (1 - \gamma_{\text{per}}^0) \chi_R (1 - \gamma_{\text{per}}^0) \\ Y_R &= \gamma_{\text{per}}^0 \eta_R \gamma_{\text{per}}^0 + (1 - \gamma_{\text{per}}^0) \eta_R (1 - \gamma_{\text{per}}^0) \end{aligned} \quad (3.11)$$

that have the virtue of commuting with the spectral projectors γ_{per}^0 and $(1 - \gamma_{\text{per}}^0)$. Note that in [2], the choice $X_R = \sqrt{1 - Y_R^2}$ is made. Here we change a bit the strategy and we only have

$$X_R^2 + Y_R^2 \leq 1.$$

Using Lemma 10 in [2], it can actually be shown that $X_R^2 + Y_R^2 \geq 1 - C/R$ for R large enough.

As noticed first in [11], the main advantage of these localization operators is that they preserve the constraint. Simply, using that $X_R \gamma_{\text{per}}^0 X_R = \gamma_{\text{per}}^0 \chi_R \gamma_{\text{per}}^0 \chi_R \gamma_{\text{per}}^0 \leq \gamma_{\text{per}}^0 (\chi_R)^2 \gamma_{\text{per}}^0 \leq \gamma_{\text{per}}^0$ and the similar estimate $X_R (1 - \gamma_{\text{per}}^0) X_R \leq 1 - \gamma_{\text{per}}^0$, we see that when $-\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0$, then

$$-\gamma_{\text{per}}^0 \leq -X_R \gamma_{\text{per}}^0 X_R \leq X_R Q X_R \leq X_R (1 - \gamma_{\text{per}}^0) X_R \leq (1 - \gamma_{\text{per}}^0).$$

These localization operators will be used to localize the kinetic energy, i.e. write it as the sum of the kinetic energies of $X_R Q_n X_R$ and $Y_R Q_n Y_R$ plus errors. As we have already used the localization functions χ_R and η_R to deal with the Coulomb terms, we also have to relate $\rho_{X_R Q X_R}$ to $\rho_{\chi_R Q \chi_R}$ and $\rho_{Y_R Q Y_R}$ to $\rho_{\eta_R Q \eta_R}$. These two tasks require the following lemma, whose proof will be detailed in the Appendix (it is based on several estimates from [2]).

Lemma 3.9 (Properties of the localization operators X_R and Y_R).

There exists a universal constant $C > 0$ such that

$$\left| \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) Q - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) X_R Q X_R - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) Y_R Q Y_R \right| \leq \frac{C}{R^2} \|Q\|_{\mathcal{Q}}, \quad (3.12)$$

$$\|\chi_R Q \chi_R - X_R Q X_R\|_{\mathcal{Q}} + \|\eta_R Q \eta_R - Y_R Q Y_R\|_{\mathcal{Q}} \leq \frac{C}{R} \|Q\|_{\mathcal{Q}}, \quad (3.13)$$

and

$$\|\rho_{\chi_R Q \chi_R} - \rho_{X_R Q X_R}\|_{L^2 \cap \mathcal{C}} + \|\rho_{\eta_R Q \eta_R} - \rho_{Y_R Q Y_R}\|_{L^2 \cap \mathcal{C}} \leq \frac{C}{R} \|Q\|_{\mathcal{Q}} \quad (3.14)$$

for all $Q \in \mathcal{Q}$.

Using (3.14) and the facts that Q_n is bounded in \mathcal{Q} and $\rho_n - \rho$ is bounded in \mathcal{C} , we get

$$\left| D(\rho_{\eta_R Q_n \eta_R}, \rho_n - \rho) - D(\rho_{Y_R Q_n Y_R}, \rho_n - \rho) \right| \leq \frac{C}{R}$$

where C is independent of n . Similarly, using (3.14) and (3.10), we deduce that

$$\left| D(\rho_{\eta_R Q_n \eta_R}, \rho_{\eta_R Q_n \eta_R}) - D(\rho_{Y_R Q_n Y_R}, \rho_{Y_R Q_n Y_R}) \right| \leq \frac{C}{R}.$$

Now if we use (3.12) to deal with the kinetic energy, we arrive at

$$\begin{aligned} F_{\text{crys}}[\rho_n] &= \mathcal{F}_{\text{crys}}[\rho_n, Q_n] \\ &= \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) X_R Q_n X_R + \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) Y_R Q_n Y_R + D(\rho_Q, \rho) + D(\rho_{Y_R Q_n Y_R}, \rho_n - \rho) \\ &\quad + \frac{1}{2} D((\chi_R)^2 \rho_Q, (\chi_R)^2 \rho_Q) + D((\chi_R)^2 \rho_Q, (\eta_R)^2 \rho_Q) + \frac{1}{2} D(\rho_{Y_R Q_n Y_R}, \rho_{Y_R Q_n Y_R}) + \varepsilon_n(R) \\ &\geq \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) X_R Q_n X_R + F_{\text{crys}}[\rho_n - \rho] + D(\rho_Q, \rho) \\ &\quad + \frac{1}{2} D((\chi_R)^2 \rho_Q, (\chi_R)^2 \rho_Q) + D((\chi_R)^2 \rho_Q, (\eta_R)^2 \rho_Q) + \varepsilon_n(R) \end{aligned}$$

where we have used that $Y_R Q_n Y_R$ is an admissible trial state for $\mathcal{F}_{\text{crys}}[\rho_n - \rho, Q]$, and where

$$\limsup_{n \rightarrow \infty} |\varepsilon_n(R)| \leq \frac{C}{R} \quad (3.15)$$

with a constant C that is independent of n . Passing to the liminf and using Fatou's lemma yields

$$\begin{aligned} \liminf_{n \rightarrow \infty} (F_{\text{crys}}[\rho_n] - F_{\text{crys}}[\rho_n - \rho]) &\geq \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) X_R Q X_R + D(\rho_Q, \rho) \\ &\quad + \frac{1}{2} D((\chi_R)^2 \rho_Q, (\chi_R)^2 \rho_Q) + D((\chi_R)^2 \rho_Q, (\eta_R)^2 \rho_Q) - \frac{C}{R} \end{aligned}$$

Using Lemma 3.6 we have

$$\lim_{R \rightarrow \infty} D((\chi_R)^2 \rho_Q, (\chi_R)^2 \rho_Q) = D(\rho_Q, \rho_Q) \quad \text{and} \quad \lim_{R \rightarrow \infty} D((\chi_R)^2 \rho_Q, (\eta_R)^2 \rho_Q) = 0.$$

Using Fatou's lemma again for the kinetic energy term, we arrive at the result

$$\liminf_{n \rightarrow \infty} (F_{\text{crys}}[\rho_n] - F_{\text{crys}}[\rho_n - \rho]) \geq \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F) Q + D(\rho_Q, \rho) + \frac{1}{2} D(\rho_Q, \rho_Q) \geq F_{\text{crys}}[\rho], \quad (3.16)$$

which is the lower bound corresponding to (3.9).

Step 2 : proof of Corollary 3.1 with $\rho \equiv 0$.

We pick a sequence $\rho_n \rightharpoonup 0$ and denote by (Q_n) the corresponding sequence of minimizers. Since (ρ_n) is bounded in \mathcal{C} , (Q_n) is bounded in \mathcal{Q} and, up to extraction, converges weakly to some $Q \in \mathcal{Q}$, which implies that $\rho_{Q_n} \rightharpoonup \rho_Q$ weakly in \mathcal{C} . We prove here that $Q \equiv 0$.

Thanks to the lower bound part of (3.9) we have just proved, we write

$$-\frac{1}{2} D(\rho_Q, \rho_Q) + F_{\text{crys}}[\rho_n] + o(1) \leq F_{\text{crys}}[-\rho_Q] + F_{\text{crys}}[\rho_n] + o(1) \leq F_{\text{crys}}[\rho_n - \rho_Q] \leq F_{\text{crys}}[\rho_n] - D(\rho_Q, \rho_{Q_n}),$$

using Q_n as a trial state for $F_{\text{crys}}[\rho_n - \rho_Q]$ and the simple lower bound $\mathcal{F}_{\text{crys}}[\nu, Q] \geq -\frac{1}{2} D(\nu, \nu)$.

Taking the limit $n \rightarrow \infty$ we therefore obtain $D(\rho_Q, \rho_Q) = 0$, which implies $Q = 0$.

Step 3: Upper bound. We now construct a trial state for $F_{\text{crys}}[\rho_n]$ to obtain the upper bound part of (3.9). In previous works [11, 2], the special structure of the set of admissible states was used (see the Appendix of [11]). We propose here a new method based on Lemma 3.8.

Let Q and Q_n be two minimizers for, respectively, the problems $F_{\text{crys}}[\rho]$ and $F_{\text{crys}}[\rho_n - \rho]$. Recall that they must satisfy the constraint $-\gamma_{\text{per}}^0 \leq Q, Q_n \leq 1 - \gamma_{\text{per}}^0$ and that, using Step 2, $Q_n \rightarrow 0$. Let χ_R be a localization function of compact support as before, $N \in \mathbb{N}$, $\vec{\tau} \in \mathcal{L}$ and $\eta_R = \chi_R(\cdot - N\vec{\tau})$. Consider the trial state (we use the notation of Lemma 3.8 with $\Pi = \gamma_{\text{per}}^0$)

$$Q_{N,R} := X_R Q X_R + U_{N\vec{\tau}} X_R Q_n X_R U_{N\vec{\tau}}^* = X_R Q X_R + Y_R Q_n Y_R$$

where $U_{N\vec{\tau}}$ is the translation unitary operator, which commutes with H_{per}^0 hence with γ_{per}^0 . When N is larger than twice the diameter of the support of χ_R , then $\chi_R^2 + \chi_R^2(\cdot - N\vec{\tau}) \leq 1$ and therefore we have $-\gamma_{\text{per}}^0 \leq Q_{N,R} \leq 1 - \gamma_{\text{per}}^0$, by Lemma 3.8. We deduce, using Lemma 3.9,

$$\begin{aligned} F_{\text{crys}}[\rho_n] &\leq \mathcal{F}_{\text{crys}}[\rho_n, Q_{N,R}] = \text{Tr}_0 \left((\gamma_{\text{per}}^0 - \varepsilon_F) X_R Q X_R \right) + D(\rho_n, \rho_Q) + \frac{1}{2} D(\chi_R^2 \rho_Q, \chi_R^2 \rho_Q) \\ &\quad + \text{Tr}_0 \left((\gamma_{\text{per}}^0 - \varepsilon_F) Y_R Q_n Y_R \right) + D(\rho_n - \rho, \rho_{Q_n}) + \frac{1}{2} D(\eta_R^2 \rho_{Q_n}, \eta_R^2 \rho_{Q_n}) \\ &\quad + D(\chi_R^2 \rho_Q, \eta_R^2 \rho_{Q_n}) + D(\rho, \eta_R^2 \rho_{Q_n}) - D(\eta_R^2 \rho_Q, \rho_n) - D(\rho_n - \rho, \chi_R^2 \rho_{Q_n}) + \varepsilon_n(R) \\ &\leq F_{\text{crys}}[\rho] + F_{\text{crys}}[\rho_n - \rho] + D(\chi_R^2 \rho_Q, \eta_R^2 \rho_{Q_n}) + D(\rho, \eta_R^2 \rho_{Q_n}) - D(\eta_R^2 \rho_Q, \rho_n) \\ &\quad - D(\rho_n - \rho, \chi_R^2 \rho_{Q_n}) + \varepsilon_n(R) \end{aligned}$$

where $\varepsilon_n(R)$ satisfies (3.15) and we have used the fact that $\chi_R^2, \eta_R^2, X_R^2, Y_R^2 \leq 1$ and the translation invariance of the energy. Now, $\chi_R^2 \rho_{Q_n} \rightarrow 0$ strongly because of the strong local compactness of ρ_{Q_n} (Lemma 3.7). Using also $\rho_n \rightarrow \rho$, $\rho_{Q_n} \rightarrow 0$ and Lemma 3.6 we can take first the limit $n \rightarrow \infty$ and then the limit $R \rightarrow \infty$ to conclude

$$\limsup_{n \rightarrow \infty} (F_{\text{crys}}[\rho_n] - F_{\text{crys}}[\rho] - F_{\text{crys}}[\rho_n - \rho]) \leq 0$$

and the proof of Proposition 3.1 is complete.

Step 4: End of the proof of Corollary 3.1. Let (ρ_n) be any sequence such that $\rho_n \rightarrow \rho$ weakly in \mathcal{C} , and Q_n be any associated sequence of minimizers for $\mathcal{F}_{\text{crys}}[\rho_n, \cdot]$. Extracting a subsequence we may assume that $Q_n \rightarrow Q$ in \mathcal{Q} . Coming back to the lower bound (3.16) obtained in Step 1 and using (3.9), we see that

$$F_{\text{crys}}[\rho] = \lim_{n \rightarrow \infty} (F_{\text{crys}}[\rho_n] - F_{\text{crys}}[\rho_n - \rho]) \geq \mathcal{F}_{\text{crys}}[\rho, Q] \geq F_{\text{crys}}[\rho].$$

This shows that Q minimizes $\mathcal{F}_{\text{crys}}[\rho, \cdot]$ and concludes the proof of Corollary 3.1. \square

4. Existence of small polarons: Proof of Theorem 2.1

Before turning to the more complicated case of N particles for which we have to adapt Theorem 25 in [13], we deal with the simpler one-particle case. The proof that a minimizer always exists for one particle follows from usual techniques of nonlinear analysis. In this context the most difficult is to verify the one-particle binding inequality (2.20), which we do first.

Step 1. Proof of the one-particle binding inequality

The aim of this first step is to prove the following important

Lemma 4.1 (One-particle binding).

We have

$$E(1) < E_{\text{per}} := \inf \sigma \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right). \quad (4.1)$$

Proof. Let u_{per} denote the first \mathcal{L} -periodic eigenfunction of $-\Delta/(2m) + V_{\text{per}}^0$, which is a solution of

$$\left(-\frac{\Delta}{2m} + V_{\text{per}}^0\right) u_{\text{per}} = E_{\text{per}} u_{\text{per}}. \quad (4.2)$$

We assume that u_{per} is normalized, $\int_{\Gamma} |u_{\text{per}}|^2 = 1$ where Γ is the unit cell of \mathcal{L} . Since $u_{\text{per}} \in H_{\text{per}}^2(\Gamma)$, we have also $\nu_{\text{per}} := |u_{\text{per}}|^2 \in H_{\text{per}}^2(\Gamma)$. The Fourier coefficients $(\widehat{\nu}_{\text{per}}(k))_{k \in \mathcal{L}^*}$ thus satisfy $(|k|^2 \widehat{\nu}_{\text{per}}(k))_{k \in \mathcal{L}^*} \in \ell^2(\mathcal{L}^*)$ and consequently belong to $\ell^1(\mathcal{L}^*)$:

$$\sum_{k \in \mathcal{L}^*} |\widehat{\nu}_{\text{per}}(k)| < \infty. \quad (4.3)$$

Here \mathcal{L}^* is the dual lattice of \mathcal{L} , whose unit cell will be denoted by Γ^* . We can write

$$|u_{\text{per}}(x)|^2 = \frac{1}{|\Gamma^*|} \sum_{k \in \mathcal{L}^*} \widehat{\nu}_{\text{per}}(k) e^{ik \cdot x}$$

Consider now a fixed function $\chi \in C_c^\infty(\mathbb{R}^3)$ such that $\int |\chi|^2 = 1$, and define the following test function for the variational problem $E(1)$:

$$\psi_\lambda := u_{\text{per}}(x) \chi_\lambda(x), \quad \text{with} \quad \chi_\lambda(x) := \lambda^{-3/2} \chi\left(\frac{x}{\lambda}\right). \quad (4.4)$$

The corresponding density is

$$|\psi_\lambda(x)|^2 := |u_{\text{per}}(x)|^2 |\chi_\lambda(x)|^2 = \frac{1}{|\Gamma^*|} \sum_{k \in \mathcal{L}^*} \widehat{\nu}_{\text{per}}(k) e^{ik \cdot x} |\chi_\lambda(x)|^2. \quad (4.5)$$

Remark that

$$D(|\chi_\lambda|^2 e^{ik \cdot}, |\chi_\lambda|^2 e^{ik \cdot}) = 4\pi \lambda^{-3} \int_{\mathbb{R}^3} \frac{|\widehat{|\chi|^2}(p)|^2}{|p/\lambda + k|^2} dp \underset{\lambda \rightarrow \infty}{\sim} \frac{4\pi}{\lambda^3 |k|^2} \int_{\mathbb{R}^3} |\widehat{|\chi|^2}(p)|^2 dp$$

for any $k \neq 0$. Using (4.3) and the fact that u_{per} is normalized, we deduce that

$$\| |\psi_\lambda|^2 - |\chi_\lambda|^2 \|_C = O\left(\frac{1}{\lambda^{3/2}}\right).$$

Similarly, the normalization factor is

$$\int_{\mathbb{R}^3} |u_{\text{per}}(x)|^2 |\chi_\lambda(x)|^2 dx = \frac{1}{(2\pi)^{3/2}} \sum_{k \in \mathcal{L}^*} \widehat{\nu}_{\text{per}}(k) \widehat{|\chi|^2}(\lambda k) = 1 + O\left(\frac{1}{\lambda^p}\right)$$

for all $p \in \mathbb{N}$. Of course, we have by scaling

$$D(|\chi_\lambda|^2, |\chi_\lambda|^2) = \frac{1}{\lambda} D(|\chi|^2, |\chi|^2).$$

We deduce from all this that

$$F_{\text{crys}} \left[\frac{|\psi_\lambda|^2}{\int_{\mathbb{R}^3} |\psi_\lambda|^2} \right] = F_{\text{crys}} [|\chi_\lambda|^2] + O\left(\frac{1}{\lambda^{3/2}}\right)$$

by (3.2). In Theorem 1.4 of [14] we have studied in detail the behavior of the crystal energy when the external density is very spread out. We have proved that

$$F_{\text{crys}} [|\chi_\lambda|^2] = F_{\text{crys}} [\lambda^{-3} |\chi(\cdot/\lambda)|^2] = \frac{1}{\lambda} F_{\varepsilon_M}^P [|\chi|^2] + o\left(\frac{1}{\lambda}\right) \quad (4.6)$$

where $F_{\varepsilon_M}^P$ is Pekar's effective interaction energy

$$F_{\varepsilon_M}^P [\rho] := 2\pi \int_{\mathbb{R}^3} |\widehat{\rho}(p)|^2 \left(\frac{1}{p^T \varepsilon_M p} - \frac{1}{|p|^2} \right) dp.$$

Since $\varepsilon_M > 1$, we have $F_{\varepsilon_M}^P[\rho] < 0$ for all ρ . So the exact (first order) behavior of the crystal energy for our trial state is

$$F_{\text{crys}} \left[\frac{|\psi_\lambda|^2}{\int_{\mathbb{R}^3} |\psi_\lambda|^2} \right] = \frac{F_{\varepsilon_M}^P[|\chi|^2]}{\lambda} + o_{\lambda \rightarrow \infty} \left(\frac{1}{\lambda} \right).$$

The two other terms in the energy \mathcal{E} are easier to handle. A simple computation based on the equation (4.2) of u_{per} shows that

$$\int_{\mathbb{R}^3} \frac{1}{2m} |\nabla \psi_\lambda|^2 + V_{\text{per}}^0 |\psi_\lambda|^2 = E_{\text{per}} \int_{\mathbb{R}^3} |\psi_\lambda|^2 + \frac{1}{2m} \int_{\mathbb{R}^3} |u_{\text{per}}|^2 |\nabla \chi_\lambda|^2$$

(see Lemma 2.2 in [14]). Of course,

$$\int_{\mathbb{R}^3} |u_{\text{per}}|^2 |\nabla \chi_\lambda|^2 \leq C \int_{\mathbb{R}^3} |\nabla \chi_\lambda|^2 = \frac{C}{\lambda^2} \int_{\mathbb{R}^3} |\nabla \chi|^2$$

since $u_{\text{per}} \in H_{\text{per}}^2 \subset L^\infty(\mathbb{R}^3)$. As a conclusion we have shown that

$$\mathcal{E} \left(\frac{\psi_\lambda}{\sqrt{\int_{\mathbb{R}^3} |\psi_\lambda|^2}} \right) = E_{\text{per}} + \frac{F_{\varepsilon_M}^P[|\chi|^2]}{\lambda} + o_{\lambda \rightarrow \infty} \left(\frac{1}{\lambda} \right).$$

Since $F_{\varepsilon_M}^P[|\chi|^2] < 0$, the inequality (4.1) follows. \square

Step 2. Compactness of minimizing sequences and existence of a minimizer for $N = 1$

We now turn to the proof of the other statements in Theorem 2.2 dealing with the one-particle case $E(1)$.

Let (ψ_n) be a minimizing sequence for $E(1)$. Since $0 \geq F_{\text{crys}}[|\psi|^2] \geq -D(|\psi|^2, |\psi|^2)/2$, it is easy to see that (ψ_n) is bounded in $H^1(\mathbb{R}^3)$. We define the largest mass that subsequences can have up to translations by

$$M := \sup \left\{ \int_{\mathbb{R}^3} |\psi|^2 : \exists (x_k) \subset \mathbb{R}^3, \psi_{n_k}(\cdot - x_k) \rightharpoonup \psi \text{ weakly in } H^1(\mathbb{R}^3) \right\}.$$

We know [18] that $M = 0$ if and only if $\psi_n \rightarrow 0$ strongly in $L^p(\mathbb{R}^3)$ for all $2 < p < 6$, a phenomenon that is usually called *vanishing*. But if this is the case, we get $\| |\psi_n|^2 \|_{\mathcal{C}} \rightarrow 0$ by the Hardy-Littlewood-Sobolev inequality, and therefore $F_{\text{crys}}[|\psi_n|^2] \rightarrow 0$ by (3.2). We then get $E(1) \geq E_{\text{per}} := \inf \sigma(H_{\text{per}}^0)$ which is impossible by Lemma 4.1. Thus $M > 0$.

Since $M > 0$ we can find a subsequence (denoted the same for simplicity), such that $\psi_n(\cdot - x_n) \rightharpoonup \psi \neq 0$. We can of course write $x_n = k_n + y_n$ where $k_n \in \mathcal{L}$ and $y_n \in \Gamma$. Extracting subsequences again we get $y_n \rightarrow y \in \Gamma$. Therefore $\psi_n(\cdot - k_n) \rightharpoonup \psi(\cdot + y) \neq 0$. Since our energy functional is invariant under the translations of \mathcal{L} , the new sequence $\psi_n(\cdot - k_n)$ is again a minimizing sequence. Without loss of generality we can thus assume that $\psi_n \rightharpoonup \psi \neq 0$. Now, if we can prove that $\int_{\mathbb{R}^3} |\psi|^2 = 1$, we will get strong convergence in L^2 and it is then standard to upgrade this to strong convergence in H^1 . We argue by contradiction and assume that $0 < \int_{\mathbb{R}^3} |\psi|^2 < 1$.

We will now show that the energy decouples in two pieces. Since $\psi_n \rightharpoonup \psi$ in $H^1(\mathbb{R}^3)$ we may assume that $|\psi_n|^2 \rightharpoonup |\psi|^2$ in \mathcal{C} . We then use that, by (3.9) in Proposition 3.1,

$$F_{\text{crys}}[|\psi_n|^2] \geq F_{\text{crys}}[|\psi|^2] + F_{\text{crys}}[|\psi_n|^2 - |\psi|^2] + o(1).$$

Note that

$$|\psi_n|^2 - |\psi|^2 - |\psi_n - \psi|^2 = 2\Re \bar{\psi}(\psi_n - \psi) \rightarrow 0$$

strongly in $L^1(\mathbb{R}^3)$ (we use here that $\psi_n \rightarrow \psi$ strongly in L_{loc}^2 and an $\varepsilon/2$ argument), hence in $L^{6/5}(\mathbb{R}^3)$ by interpolation. Thus

$$\lim_{n \rightarrow \infty} \left| F_{\text{crys}}[|\psi_n|^2 - |\psi|^2] - F_{\text{crys}}[|\psi_n - \psi|^2] \right| = 0$$

by (3.2) in Lemma 3.2, and we arrive at

$$F_{\text{crys}}[|\psi_n|^2] \geq F_{\text{crys}}[|\psi|^2] + F_{\text{crys}}[|\psi_n - \psi|^2] + o(1).$$

On the other hand, it is clear from the weak convergence $\psi_n \rightharpoonup \psi$ in $H^1(\mathbb{R}^3)$ (and from the fact that the form domain of $-\Delta/(2m) + V_{\text{per}}^0$ is $H^1(\mathbb{R}^3)$), that

$$\left\langle \psi_n, \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) \psi_n \right\rangle = \left\langle \psi, \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) \psi \right\rangle + \left\langle (\psi_n - \psi), \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) (\psi_n - \psi) \right\rangle + o(1).$$

Hence we have shown that

$$\mathcal{E}[\psi_n] \geq \mathcal{E}[\psi] + \mathcal{E}[\psi_n - \psi] + o(1).$$

Now we use that F_{crys} is concave to infer

$$F_{\text{crys}}[|\psi_n - \psi|^2] \geq \left(\int_{\mathbb{R}^3} |\psi_n - \psi|^2 \right) F_{\text{crys}} \left[\frac{|\psi_n - \psi|^2}{\int_{\mathbb{R}^3} |\psi_n - \psi|^2} \right],$$

leading to

$$\begin{aligned} \mathcal{E}[\psi_n] &\geq \mathcal{E}[\psi] + \left(\int_{\mathbb{R}^3} |\psi_n - \psi|^2 \right) \mathcal{E} \left[\frac{|\psi_n - \psi|^2}{\int_{\mathbb{R}^3} |\psi_n - \psi|^2} \right] + o(1) \\ &\geq \mathcal{E}[\psi] + \left(\int_{\mathbb{R}^3} |\psi_n - \psi|^2 \right) E(1) + o(1). \end{aligned}$$

Passing to the limit $n \rightarrow \infty$, we find

$$E(1) \geq \mathcal{E}[\psi] + \left(1 - \int_{\mathbb{R}^3} |\psi|^2 \right) E(1).$$

It is now time to use the strict concavity at the origin (3.1)

$$F_{\text{crys}}[|\psi|^2] > \left(\int_{\mathbb{R}^3} |\psi|^2 \right) F_{\text{crys}} \left[\frac{|\psi|^2}{\int_{\mathbb{R}^3} |\psi|^2} \right],$$

which yields

$$\mathcal{E}[\psi] > \left(\int_{\mathbb{R}^3} |\psi|^2 \right) \mathcal{E} \left[\frac{|\psi|^2}{\int_{\mathbb{R}^3} |\psi|^2} \right] \geq \left(\int_{\mathbb{R}^3} |\psi|^2 \right) E(1).$$

Therefore we have proved that $E(1) > E(1)$ which is a contradiction, unless $\int_{\mathbb{R}^3} |\psi|^2 = 1$. This concludes the proof in the case of one particle.

5. Binding of small N -polarons: Proof of Theorem 2.2

We now turn to the case of $N \geq 2$. With the input of Section 3, the proof more or less follows that of Theorem 25 in [13]. We nevertheless sketch the main steps for the convenience of the reader.

We will denote

$$H(N) := \sum_{j=1}^N \left(-\frac{\Delta_j}{2m} + V_{\text{per}}^0(x_j) \right) + \sum_{i < j} \frac{1}{|x_i - x_j|}.$$

In order to relate problems with different particle numbers to one another, it is crucial to introduce the antisymmetric truncated Fock space

$$\mathcal{F}^{\leq N} = \bigoplus_{n=0}^N \bigwedge_{i=1}^n L^2(\mathbb{R}^3)$$

where \bigwedge is the antisymmetric tensor product and we use the convention $\bigwedge_{i=1}^0 L^2(\mathbb{R}^3) = \mathbb{C}$. A state on $\mathcal{F}^{\leq N}$ is an operator $\Gamma \in \mathfrak{S}^1(\mathcal{F}^{\leq N})$ with $\text{Tr}(\Gamma) = 1$. In the sequel we restrict ourselves to states commuting with the number operator

$$\mathcal{N} = \bigoplus_{n=0}^N n.$$

This means (see [13], Remark 7) that they take the form

$$\Gamma = G_{00} \oplus \dots \oplus G_{NN} \quad (5.1)$$

with $G_{ii} \in \mathfrak{S}^1(\bigwedge_{i=1}^n L^2(\mathbb{R}^3))$. We denote by

$$\mathbb{H} = \bigoplus_{n=0}^N H(n)$$

the many-body second-quantized Hamiltonian. To any state Γ are associated a density $\rho_\Gamma \in L^1(\mathbb{R}^3)$, one-body density matrix $[\Gamma]^{1,1} \in \mathfrak{S}^1(L^2(\mathbb{R}^3))$ and two-body density matrix $[\Gamma]^{2,2} \in \mathfrak{S}^1(L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3))$ (see [13], Section 1). We can extend the energy to Fock space as

$$\begin{aligned} \mathcal{E}[\Gamma] &= \text{Tr}_{\mathcal{F}^{\leq N}}(\mathbb{H}\Gamma) + F_{\text{crys}}[\rho_\Gamma] \\ &= \text{Tr}_{L^2(\mathbb{R}^3)}((-\Delta + V_{\text{per}}^0)[\Gamma]^{1,1}) + \text{Tr}_{L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3)}(W[\Gamma]^{2,2}) + F_{\text{crys}}[\rho_\Gamma] \end{aligned}$$

where W acts on $L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ as the multiplication by $|x - y|^{-1}$. For a pure state $\Gamma = 0 \oplus \dots \oplus |\Psi\rangle\langle\Psi|$ with $\Psi \in L^2(\mathbb{R}^{3N})$ one can check that $\mathcal{E}[\Gamma] = \mathcal{E}[\Psi]$. More generally, for a state of the form (5.1), we have

$$\mathcal{E}[\Gamma] = \sum_{n=1}^N \text{Tr}_{\bigwedge_1^n L^2(\mathbb{R}^3)}(H(n)G_{nn}) + F_{\text{crys}}\left[\sum_{n=1}^N \rho_{G_{nn}}\right].$$

Step 1. Large binding inequality.

We claim that

$$E(N) \leq E(N - k) + E(k) \text{ for all } k = 1, \dots, N - 1. \quad (5.2)$$

To see this, we consider the following trial state:

$$\Psi_R^N := \Psi^{N-k} \wedge \Psi^k(\cdot - R\vec{\tau}) \quad (5.3)$$

where (Ψ^{N-k}) and (Ψ^k) are compactly supported fixed trial states for $E(N - k)$ and $E(k)$ respectively, $\vec{\tau} \in \mathcal{L}$ is a lattice translation and $R \in \mathbb{N}$ is large enough for $\rho_{\Psi^{N-k}}$ and $\rho_{\Psi^k}(\cdot - R\vec{\tau})$ to have disjoint supports. The symbol \wedge denotes the antisymmetric tensor product. We first take the limit $R \rightarrow \infty$ to obtain

$$E(N) \leq \mathcal{E}[\Psi^{N-k}] + \mathcal{E}[\Psi^k]. \quad (5.4)$$

Optimizing then with respect to Ψ^{N-k} and Ψ^k concludes the proof of (5.2). To see that (5.4) holds, we note that by construction

$$\rho_{\Psi_R^N} = \rho_{\Psi^{N-k}} + \rho_{\Psi^k}(\cdot - R\vec{\tau})$$

for large enough R , thus we can use Proposition 3.1 and take the limit $R \rightarrow \infty$ with $R \in \mathbb{N}$ to obtain

$$\lim_{R \rightarrow \infty} F_{\text{crys}}[\rho_{\Psi_R^N}] = F_{\text{crys}}[\rho_{\Psi^{N-k}}] + F_{\text{crys}}[\rho_{\Psi^k}].$$

The other terms in the energy can be treated as usual to obtain (5.4).

Note that the argument here also proves by contradiction that Item (2) of Theorem 2.2 implies Item (1). If there is equality in (5.2), we can choose Ψ_n^{N-k} and Ψ_n^k minimizing sequences for $E(N - k)$ and $E(k)$ respectively and, taking $R_n \rightarrow \infty$ very fast, we obtain a minimizing sequence for $E(N)$ that is not precompact, even up to translations because some mass is lost at infinity.

Step 2. Absence of vanishing.

We consider a minimizing sequence (Ψ_n) for $E(N)$ and denote by $\Gamma_n = 0 \oplus \dots \oplus |\Psi_n\rangle \langle \Psi_n|$ the associated state in the truncated antisymmetric Fock space. It is easy to see, using in particular Lemma 3.2 that (Ψ_n) is bounded in $H^1(\mathbb{R}^{3N})$. As in the one-body case treated before, we define a criterion for the vanishing of the minimizing sequence. We use the concept of geometric convergence (see Section 2 in [13] for the definition). We look at the the mass of the possible geometric limits, up to translations and extraction, of (Γ_n)

$$M := \sup \left\{ \text{Tr}(\mathcal{N}\Gamma), \exists \vec{v}_k \subset \mathbb{R}^3, \vec{v}_k \Gamma_{n_k} \vec{v}_k^* \rightharpoonup_g \Gamma \right\}$$

where we recall that \mathcal{N} is the number operator in Fock space. As explained in [13], Lemma 24, if $M = 0$ then $\rho_{\Psi_n} \rightarrow 0$ strongly in $L^p(\mathbb{R}^3)$ for all $1 < p < 3$. Using then Lemma 3.2 we obtain $F_{\text{crys}}[\rho_{\Psi_n}] \rightarrow 0$ and therefore

$$E(N) = \lim_{n \rightarrow \infty} \mathcal{E}[\Psi_n] \geq \inf \sigma \left(\tilde{H}(N) \right) = NE_{\text{per}}$$

where

$$\tilde{H}(N) := \sum_{j=1}^N \left(-\frac{\Delta_j}{2m} + V_{\text{per}}^0(x_j) \right) = \sum_{j=1}^N (H_{\text{per}}^0)_{x_j}. \quad (5.5)$$

Note that, by induction on N , (5.2) implies $E(N) \leq NE(1)$. We have already seen in (4.1) above that $E(1) < \inf \sigma(H_{\text{per}}^0)$. Hence we reach a contradiction and conclude that $M > 0$.

Step 3. Decoupling via localization

Since $M > 0$ (and arguing as in the previous section) we have, up to the extraction of a subsequence, $\vec{v}_n \Gamma_n \vec{v}_n^* \rightharpoonup_g \Gamma$ with $\text{Tr}(\mathcal{N}\Gamma) > 0$ and where $(\vec{v}_n) \subset \mathcal{L}$ is a sequence of lattice translations. Using the invariance of the energy, Lemma 3.3, we can thus assume that our minimizing sequence satisfies

$$\Gamma_n \rightharpoonup_g \Gamma \quad (5.6)$$

with $\text{Tr}(\mathcal{N}\Gamma) > 0$. Also we have $\sqrt{\rho_{\Gamma_n}} \rightharpoonup \sqrt{\rho_\Gamma}$ weakly in $H^1(\mathbb{R}^3)$ and strongly in L_{loc}^2 . Also $\rho_{\Gamma_n} \rightharpoonup \rho_\Gamma$ in the Coulomb space \mathcal{C} and we immediately deduce by (3.9) that

$$F_{\text{crys}}[\rho_{\Gamma_n}] \geq F_{\text{crys}}[\rho_\Gamma] + F_{\text{crys}}[\rho_{\Gamma_n} - \rho_\Gamma] + o(1).$$

We now pick a sequence of radii $R_n \rightarrow \infty$ and define smooth localization functions χ_{R_n} and η_{R_n} such that $\chi_{R_n}^2 + \eta_{R_n}^2 = 1$, $\text{supp}(\chi_{R_n}) \subset B(0, 2R_n)$ and $\text{supp}(\eta_{R_n}) \subset \mathbb{R}^3 \setminus B(0, 3R_n)$. For any bounded operator B (in particular the multiplication by a function χ) on $L^2(\mathbb{R}^3)$ such that $0 \leq BB^* \leq 1$ we will denote by $(\Gamma)_B$ the B -localization of a state Γ , as defined in [13], Section 3. Of importance to us will be the following properties of localization:

$$\begin{aligned} \rho_{\Gamma_\chi} &= \chi^2 \rho_\Gamma \\ [\Gamma_\chi]^{1,1} &= \chi [\Gamma]^{1,1} \chi \\ [\Gamma_\chi]^{2,2} &= \chi \otimes \chi [\Gamma]^{2,2} \chi \otimes \chi. \end{aligned} \quad (5.7)$$

Also, for a state of the form (5.1), writing

$$(\Gamma)_{\chi_{R_n}} = G_0^{\chi_{R_n}} \oplus \dots \oplus G_N^{\chi_{R_n}}, \quad (\Gamma)_{\eta_{R_n}} = G_0^{\eta_{R_n}} \oplus \dots \oplus G_N^{\eta_{R_n}},$$

the condition $\chi_{R_n}^2 + \eta_{R_n}^2 = 1$ implies the relation

$$\text{Tr}(G_j^{\chi_{R_n}}) = \text{Tr}(G_{N-j}^{\eta_{R_n}}). \quad (5.8)$$

Using concentration functions as in Step 4 of the proof of [13], Theorem 25 we have, extracting a further subsequence if necessary

$$(\Gamma_n)_{\chi_{R_n}} \rightarrow \Gamma \text{ strongly in } \mathfrak{S}^1(\mathcal{F}^{\leq N}) \quad (5.9)$$

and

$$(\chi_{R_n})^2 \rho_{\Gamma_n} \rightarrow \rho_\Gamma \text{ strongly in } L^p(\mathbb{R}^3) \text{ for all } 2 \leq p < 3. \quad (5.10)$$

Using (3.2), this can be used to prove that

$$F_{\text{crys}}[\rho_{\Gamma_n} - \rho_\Gamma] = F_{\text{crys}}[(\eta_{R_n})^2 \rho_{\Gamma_n}] + o(1).$$

Thus

$$F_{\text{crys}}[\rho_{\Gamma_n}] \geq F_{\text{crys}}[\rho_\Gamma] + F_{\text{crys}}[\rho_{(\Gamma_n)_{\eta_{R_n}}}] + o(1).$$

We have seen that the nonlinear energy F_{crys} decouples. The other terms are treated following [13]. For the one-particle part we use the IMS formula

$$\Delta = \chi_{R_n} \Delta \chi_{R_n} + \eta_{R_n} \Delta \eta_{R_n} + |\nabla \chi_{R_n}|^2 + |\nabla \eta_{R_n}|^2$$

to obtain (we use (5.7))

$$\begin{aligned} \text{Tr} \left(\left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) [\Gamma_n]^{(1,1)} \right) &\geq \text{Tr} \left(\chi_{R_n} \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) \chi_{R_n} [\Gamma_n]^{(1,1)} \right) \\ &\quad + \text{Tr} \left(\eta_{R_n} \left(-\frac{\Delta}{2m} + V_{\text{per}}^0 \right) \eta_{R_n} [\Gamma_n]^{(1,1)} \right) - \frac{CN}{R_n^2} \\ &= \text{Tr}(\mathbb{H}(\Gamma_n)_{\chi_{R_n}}) + \text{Tr}(\mathbb{H}(\Gamma_n)_{\eta_{R_n}}) - \frac{CN}{R_n^2}. \end{aligned}$$

The Coulomb interaction is treated exactly as in [13] and we conclude

$$\langle \Psi_n, H(N) \Psi_n \rangle \geq \text{Tr}(\mathbb{H}(\Gamma_n)_{\chi_{R_n}}) + \text{Tr}(\mathbb{H}(\Gamma_n)_{\eta_{R_n}}) + o(1).$$

Using Fatou's lemma as well as the strong convergence of $(\chi_{R_n})^2 \rho_{\Gamma_n}$, we finally get

$$\mathcal{E}[\Psi_n] \geq \mathcal{E}[\Gamma] + \mathcal{E}[(\Gamma_n)_{\eta_{R_n}}] + o(1). \quad (5.11)$$

which is the desired decoupling of the energy.

Step 4. Conclusion.

The rest of the argument follows exactly [13]. Writing the geometric limit of Γ_n

$$\Gamma = G_{00} \oplus \dots \oplus G_{NN},$$

and using the concavity of F_{crys} , the fundamental relation (5.8) as well as the convergence (5.9), we arrive at

$$E(N) \geq \sum_{j=0}^N \text{Tr}(G_{jj}) (E(j) + E(N-j)).$$

Assuming the strict binding inequalities (2.21), this is possible only when $G_{11} = \dots = G_{N-1N-1} = 0$. Hence we necessarily have $G_{NN} \neq 0$, otherwise we would obtain a contradiction with the fact that $\text{Tr}(\mathcal{N}\Gamma) > 0$.

To conclude, it is then enough to prove that $G_{00} = 0$, which is an easy consequence of the strict concavity (3.1) of F_{crys} (see Step 5 of the proof of Theorem 25 in [13] for details). We deduce that $\text{Tr}(G_{NN}) = 1 = \text{Tr}(|\Psi_n\rangle \langle \Psi_n|)$, hence that the weak-* convergence of $|\Psi_n\rangle \langle \Psi_n|$ in $\mathfrak{S}^1(L^2(\mathbb{R}^3))$ to G_{NN} is actually strong because no mass is lost in the weak limit. As $G_{NN} = |\Psi\rangle \langle \Psi|$ where Ψ is the weak limit of Ψ_n , we conclude that Ψ_n converges to Ψ strongly in $L^2(\mathbb{R}^3)$. The convergence in $H^1(\mathbb{R}^3)$ follows by standard arguments. \square

Appendix. Proof of Lemma 3.9

We follow ideas of [2]. We start with the second estimate (3.13) of Lemma 3.9, and write for instance

$$\begin{aligned} (X_R Q X_R - \chi_R Q \chi_R)^{-} &= X_R Q^{-} X_R - \chi_R Q^{-} \chi_R - [\gamma_{\text{per}}^0, \chi_R] Q \chi_R \gamma_{\text{per}}^0 - \chi_R \gamma_{\text{per}}^0 Q [\chi_R, \gamma_{\text{per}}^0] \\ &= (X_R - \chi_R) Q^{-} X_R + \chi_R Q^{-} (X_R - \chi_R) \\ &\quad - [\gamma_{\text{per}}^0, \chi_R] Q \chi_R \gamma_{\text{per}}^0 - \chi_R \gamma_{\text{per}}^0 Q [\chi_R, \gamma_{\text{per}}^0]. \end{aligned} \quad (5.12)$$

When we multiply by $|H_{\text{per}}^0 - \varepsilon_F|^{1/2}$ on both sides, we have to estimate several terms. For the last one we write

$$\begin{aligned} &|H_{\text{per}}^0 - \varepsilon_F|^{1/2} \chi_R \gamma_{\text{per}}^0 Q [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \\ &= \left[|H_{\text{per}}^0 - \varepsilon_F|^{1/2}, \chi_R \right] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \gamma_{\text{per}}^0 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \\ &\quad + \chi_R \gamma_{\text{per}}^0 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2}. \end{aligned} \quad (5.13)$$

In Lemma 10 of [2] it is proved that $\|[\chi_R, \gamma_{\text{per}}^0]\|_{\mathfrak{S}^2} = O(R^{-1})$ and the same proof can be employed to show that

$$\left\| [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\|_{\mathfrak{S}^2} = O\left(\frac{1}{R}\right)$$

as well. Also, following the proof of Lemma 11 of [2], one can show that

$$\left\| \left[|H_{\text{per}}^0 - \varepsilon_F|^{1/2}, \chi_R \right] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| \leq C R^{-1}.$$

For the first term of the right-hand side of (5.13) we can thus write

$$\begin{aligned} &\left\| \left[|H_{\text{per}}^0 - \varepsilon_F|^{1/2}, \chi_R \right] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \gamma_{\text{per}}^0 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\| \\ &\leq \left\| \left[|H_{\text{per}}^0 - \varepsilon_F|^{1/2}, \chi_R \right] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| \left\| \gamma_{\text{per}}^0 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q \right\|_{\mathfrak{S}^2} \left\| [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\|_{\mathfrak{S}^2} \leq C R^{-2}. \end{aligned}$$

We turn to the second term. Using that $|H_{\text{per}}^0 - \varepsilon_F|^{1/2}(1 - \Delta)^{-1/2}$ and its inverse are bounded by Lemma 1 in [2], we see that

$$\left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q \right\|_{\mathfrak{S}^2} \leq C \left\| (1 - \Delta)^{1/2} Q \right\|_{\mathfrak{S}^2} \leq C \|Q\|_{\mathcal{Q}}.$$

So we get

$$\left\| \chi_R \gamma_{\text{per}}^0 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} Q [\chi_R, \gamma_{\text{per}}^0] |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\|_{\mathfrak{S}^1} \leq \frac{C \|Q\|_{\mathcal{Q}}}{R}.$$

Then, for the first terms in (5.12), we use that

$$\begin{aligned} &\left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} (X_R - \chi_R) Q^{-} X_R |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\|_{\mathfrak{S}^1} \\ &\leq C \|Q\|_{\mathcal{Q}} \left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} (X_R - \chi_R) |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| \left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} X_R |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\|. \end{aligned}$$

Of course we have

$$|H_{\text{per}}^0 - \varepsilon_F|^{1/2} X_R |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} = \left[|H_{\text{per}}^0 - \varepsilon_F|^{1/2}, X_R \right] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} + X_R$$

and a similar formula for $X_R - \chi_R$. The first commutator is a $O(R^{-1})$ by Lemma 11 in [2]. Also we have $\|X_R - \chi_R\| = O(R^{-1})$ by Lemma 10 in [2]. In total, we have actually shown that

$$\left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} (X_R Q X_R - \chi_R Q \chi_R)^{-} |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\|_{\mathfrak{S}^1} \leq \frac{C \|Q\|_{\mathcal{Q}}}{R}.$$

In order to conclude the proof of (3.13) we still have to show that

$$\left\| |H_{\text{per}}^0 - \varepsilon_F|^{1/2} (X_R Q X_R - \chi_R Q \chi_R) \right\|_{\mathfrak{S}^2} \leq \frac{C \|Q\|_{\mathcal{Q}}}{R}. \quad (5.14)$$

The proof of this is similar but simpler and we omit the details.

By Proposition 1 of [2], we know that the linear map $Q \in \mathcal{Q} \mapsto \rho_Q \in \mathcal{C} \cap L^2$ is continuous. So the third estimate (3.14) in the statement simply follows from the estimate (3.13) on the norm of \mathcal{Q} .

It remains to discuss the kinetic energy estimate (3.12) in Lemma 3.9. First we remark that

$$(\chi_R^2)^{--} = \gamma_{\text{per}}^0 \chi_R (\gamma_{\text{per}}^0 + (\gamma_{\text{per}}^0)^\perp) \chi_R \gamma_{\text{per}}^0 = (X_R^2)^{--} + [\gamma_{\text{per}}^0, \chi_R] (\gamma_{\text{per}}^0)^\perp [\chi_R, \gamma_{\text{per}}^0]$$

and a similar equality for $(\chi_R^2)^{++}$. Since by construction

$$X_R^2 = (X_R^2)^{++} + (X_R^2)^{--}$$

this yields

$$(\chi_R^2)^{--} + (\chi_R^2)^{++} = X_R^2 - [\gamma_{\text{per}}^0, \chi_R]^2 \quad \text{and} \quad (\eta_R^2)^{--} + (\eta_R^2)^{++} = Y_R^2 - [\gamma_{\text{per}}^0, \eta_R]^2.$$

From this we deduce that

$$\begin{aligned} \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Q &= \text{Tr}(H_{\text{per}}^0 - \varepsilon_F)(Q^{++} + Q^{--}) \\ &= \text{Tr} \frac{(\chi_R^2 + \eta_R^2)(H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)(\chi_R^2 + \eta_R^2)}{2} (Q^{++} + Q^{--}) \\ &= \text{Tr} \frac{(X_R^2 + Y_R^2)(H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)(X_R^2 + Y_R^2)}{2} (Q^{++} + Q^{--}) \\ &\quad - \text{Tr} \frac{[\gamma_{\text{per}}^0, \chi_R]^2 (H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)[\gamma_{\text{per}}^0, \chi_R]^2}{2} (Q^{++} + Q^{--}) \\ &\quad - \text{Tr} \frac{[\gamma_{\text{per}}^0, \eta_R]^2 (H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)[\gamma_{\text{per}}^0, \eta_R]^2}{2} (Q^{++} + Q^{--}) \end{aligned}$$

hence that

$$\begin{aligned} \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Q - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)X_R Q X_R - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Y_R Q Y_R \\ = \frac{1}{2} \text{Tr} ([X_R, [X_R, H_{\text{per}}^0]] + [Y_R, [Y_R, H_{\text{per}}^0]])(Q^{++} + Q^{--}) \\ - \frac{1}{2} \text{Tr} ([\gamma_{\text{per}}^0, \chi_R]^2 (H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)[\gamma_{\text{per}}^0, \chi_R]^2)(Q^{++} + Q^{--}) \\ - \frac{1}{2} \text{Tr} ([\gamma_{\text{per}}^0, \eta_R]^2 (H_{\text{per}}^0 - \varepsilon_F) + (H_{\text{per}}^0 - \varepsilon_F)[\gamma_{\text{per}}^0, \eta_R]^2)(Q^{++} + Q^{--}). \end{aligned}$$

We conclude that

$$\begin{aligned} |\text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Q - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)X_R Q X_R - \text{Tr}_0(H_{\text{per}}^0 - \varepsilon_F)Y_R Q Y_R| \\ \leq C \|Q\|_{\mathcal{Q}} \left(\left\| |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} [X_R, [X_R, H_{\text{per}}^0]] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| \right. \\ \left. + \left\| |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} [Y_R, [Y_R, H_{\text{per}}^0]] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| \right. \\ \left. + \left\| [\gamma_{\text{per}}^0, \chi_R]^2 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\| + \left\| [\gamma_{\text{per}}^0, \eta_R]^2 |H_{\text{per}}^0 - \varepsilon_F|^{1/2} \right\| \right). \end{aligned}$$

The last two error terms can be estimated by arguing as before, using (5.14). For the double commutators, a computation shows that

$$\begin{aligned} [X_R, [X_R, H_{\text{per}}^0]] &= (\gamma_{\text{per}}^0)^\perp \left([\chi_R, \gamma_{\text{per}}^0] [\chi_R, \Delta] + [\chi_R, \Delta] [\chi_R, \gamma_{\text{per}}^0] + |\nabla \chi_R|^2 \right) (\gamma_{\text{per}}^0)^\perp \\ &\quad - \gamma_{\text{per}}^0 \left([\chi_R, \gamma_{\text{per}}^0] [\chi_R, \Delta] + [\chi_R, \Delta] [\chi_R, \gamma_{\text{per}}^0] + |\nabla \chi_R|^2 \right) \gamma_{\text{per}}^0. \end{aligned}$$

We have $[\chi_R, \Delta] = (\Delta \chi_R) + 2i \nabla \chi \cdot p$ with $p = -i \nabla$. Using then that $p |H_{\text{per}}^0 - \varepsilon_F|^{-1/2}$ is bounded and the fact that $\|[\chi_R, \gamma_{\text{per}}^0]\| = O(R^{-1})$, we conclude similarly as before that

$$\left\| |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} [X_R, [X_R, H_{\text{per}}^0]] |H_{\text{per}}^0 - \varepsilon_F|^{-1/2} \right\| = O\left(\frac{1}{R^2}\right).$$

The term involving Y_R is treated similarly. This ends our proof of the first estimate (3.12), hence the proof of Lemma 3.9. \square

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